

# **A Rapid Genetic Optimization Technique for Rational Thermodynamic Modeling Having Reliable Third Virial Coefficients**

I.M. Astina<sup>C, S</sup>

*School of Science for Open and Environmental Systems, Keio University, Yokohama, Japan*

H. Sato

*Faculty of Science and Technology, Keio University, Yokohama, Japan*

Two important aspects for developing thermodynamic equations of state (EOS) for fluids are the modeling technique to achieve an effective and reliable computational process and the theoretical background for comprehensive rational thermodynamic modeling to represent reliable thermodynamic properties. Although existing EOS's for hydrofluorocarbons (HFC) are believed to be highly reliable, our group pointed out three years ago that the specific heat values derived from the existing Helmholtz EOS's do not agree with each other in the gaseous phase, and the maximum deviation appears at saturation as being more than 5 % in the worst case. Those EOS were developed mostly on the basis of experimental data. Especially in the low-temperature gaseous phase where refrigeration systems are working, very limited or no data for HFC's are available. Therefore, a Helmholtz EOS should be developed not only based on reliable experimental data but also on the theoretical background.

Regarding the modeling technique, several genetic operators have been already introduced to the optimization procedures of many researchers. In practice, those are not perfectly completed in the applications due to unresolved constraints and complicated targets. Learning the performance of the operators and their arrangements is an important task to find a shorter computational optimization process and the result to remain being highly accurate. Owing to the Gaussian distribution as natural evolutionary process model and the biology principle, several types of genetic operators were introduced in a series of process, recombination, mutation, survival, and selection. A new qualitative and quantitative procedure will be proposed for the selection and assessment of thermodynamic property modeling for fluids.

As a result of the new modeling technique and the consideration of theoretical background, Helmholtz EOS which can provide reliable third virial coefficient will be demonstrated for several HFC's. Comprehensive analyses for significance of the third virial coefficient on thermodynamic property modeling will be also discussed.